Combinatorial Discovery of Chemicals and Materials

An ATP Focused Program for FY 1999

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Visit us at: http://www.atp.nist.gov/www/ccmr/ccmr_off.htm

Agenda

- The Advanced Technology Program
  - *We Fund Research in High-Risk Technologies*
- Combinatorial Methods of Discovery
  - *Significant Technology Entry Barriers*
- The Opportunity for ATP in Combi chem
  - *We’re Looking For a Few Good Risks*

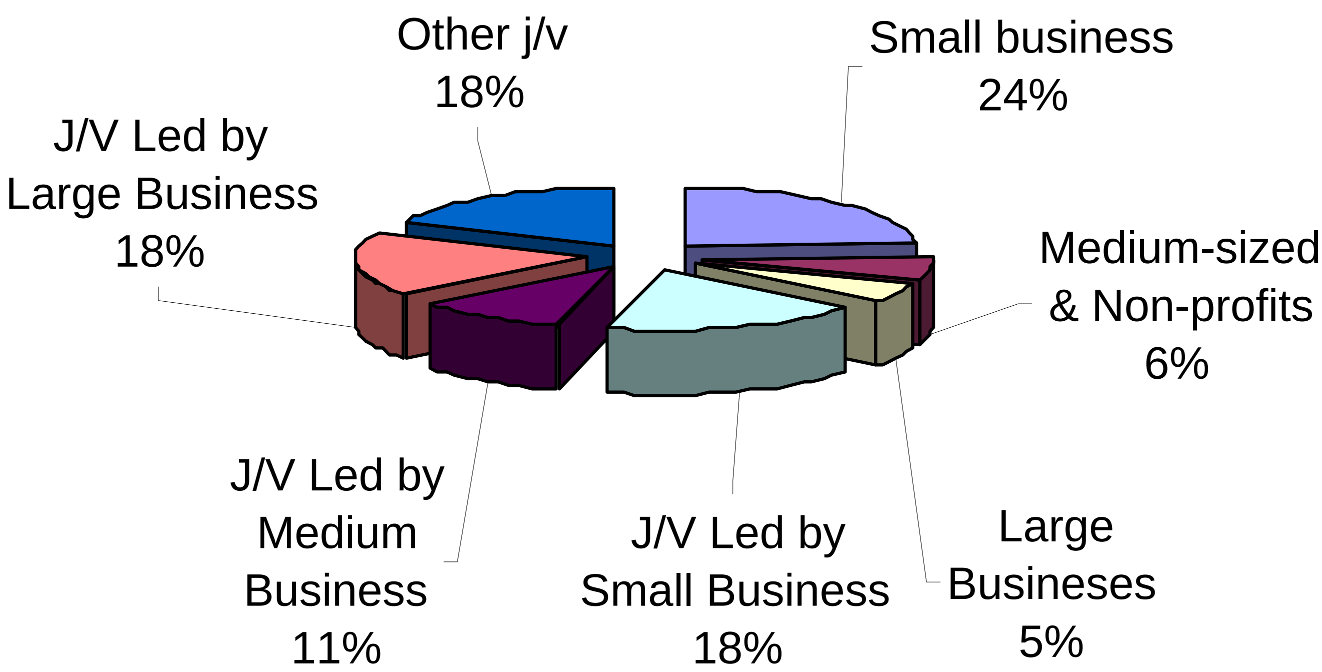
$ 66,000,000

A total estimated $66 million in first year funding for fiscal year 1999 is expected to become available from Congressional appropriation for new awards. The actual number of fiscal year 1999 proposals funded will depend on the quality of the proposals received and the amount of funding requested in the highest ranked proposals. Outyear funding beyond the first year is contingent on the approval of future Congressional appropriations and satisfactory project performance. Only full proposals are being solicited under this single competition, however, abbreviated proposals (pre-proposals) may be submitted and are optional.

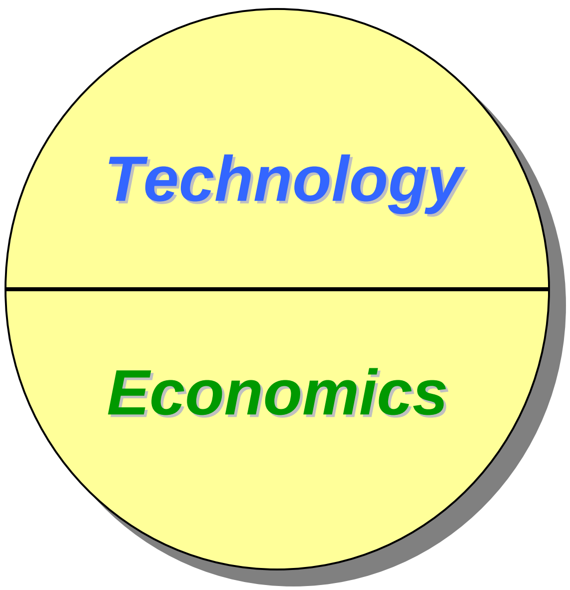
What is the NIST ATP?

- Industry driven (U.S. Dept. of Commerce)
- Opens new opportunities for U.S. industry
- Different from other government programs
  - *Intell. Prop. retained by industrial awardees*
  - *~50% cost-share (depends on company size)*
  - *Confidential proposals and reporting (no FOIA)*

Distribution of $1,386 M to 431 ATP Awards (1990 - 1998)



What We Look For in a Proposal



50% Scientific and Technological Merit

- *Innovations in the Technology*
- *High Technical Risk & Feasibility*
- *Quality of R&D Plan*

50% Broad-Based Economic Benefits

- *Economic Benefits*
- *Need for ATP funding*
- *Pathway to Economic Benefit*

No Proposal will be Funded That Does Not Have High Scientific and Technical Merit

Our Targets: Where Market Needs and Technologies Converge

- Markets demand higher performance/price ratios
- Globalization of markets increases *pace* of change

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- Convergence of hardware and software technologies
- Lower cost, generic solutions increase availability

COMBINATORIAL CHEMISTRY

Chemicals and materials sectors have unique drivers...

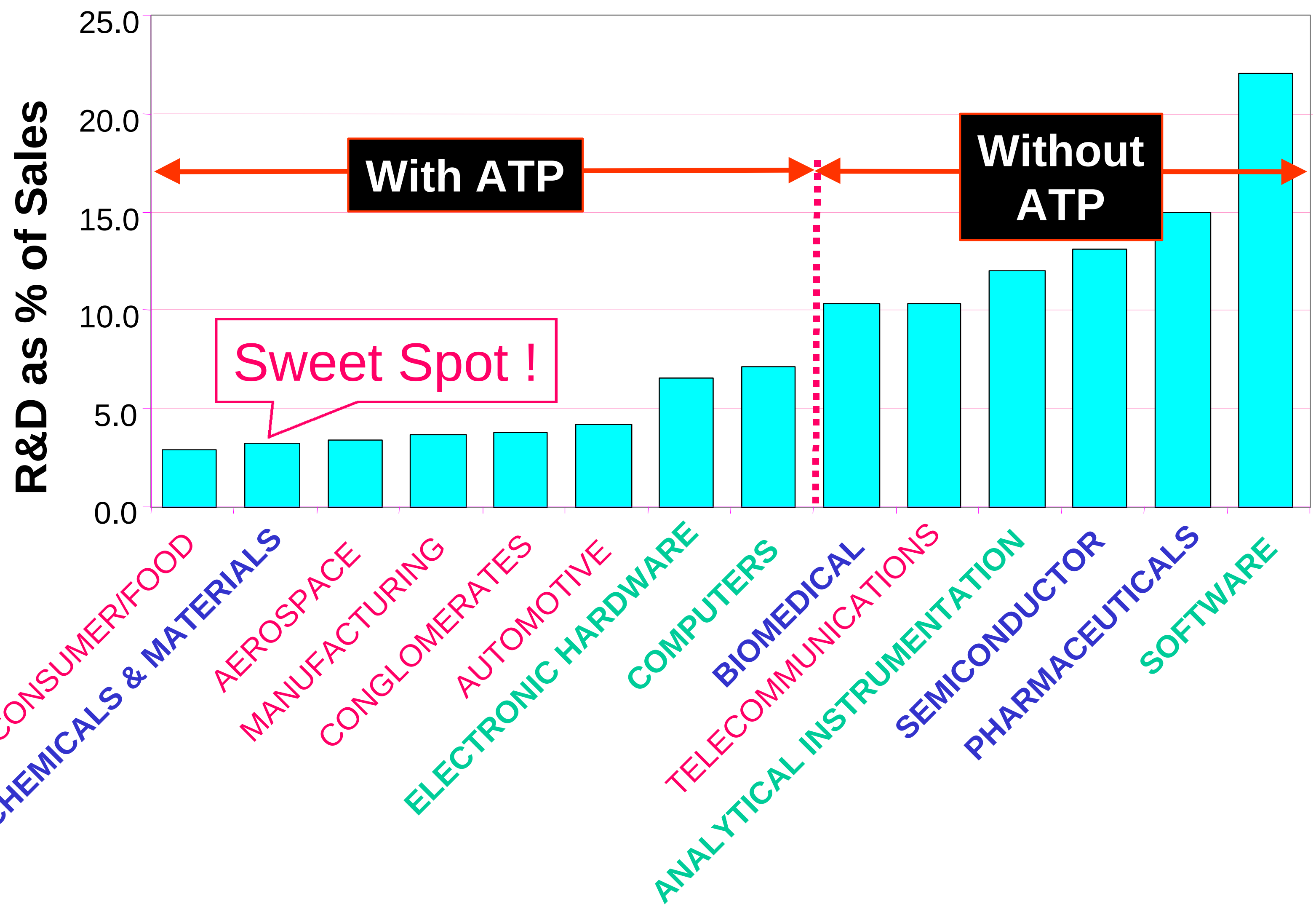
- *Low investment in non-core technologies or businesses*
- *Long pay-back of R&D capital investment (R&D ROI)*
- *Difficult displacement of installed R&D or mfg. assets is (ROA)*
- *Leverage of commodity/specialty materials profits (8%/15%)*

especially with respect to combinatorial methodologies

- *Integration of new base technologies and systems*
- *Significant technological hurdles in materials discovery and process/product development with current technology*
- *Cultural barriers*

Combinatorial Chemistry

Where can ATP make a difference?



Opportunities and Issues

Polymers: $38B industry with $1.5B in R&D

• *Engineering, commodity, blends and alloys, bio-compatibles*

• *Sensors for mechanical properties and bio-compatibilty*

? *Scalability: bulk- and processing-dependent properties*

Electronic/Photonic Materials: $HUGE

• *Lighting, display materials, dielectrics, semi-conductors, wave guides*

• *Lowered energy consumption, environmental impact*

? *Sample purity, spectral analyses, substrate interactions (scalability)*

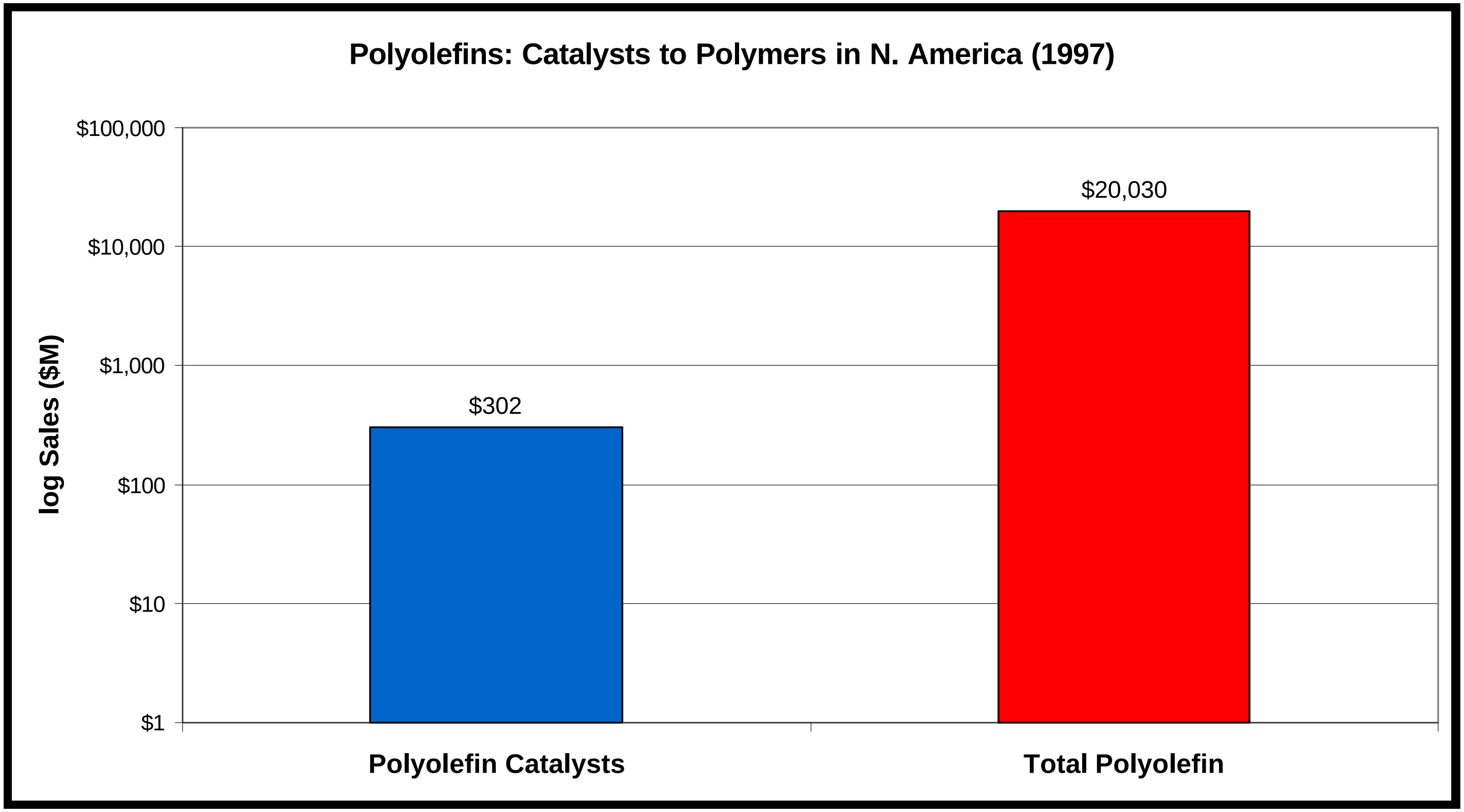
Catalysts: $10B catalyst industry, $12B R&D (incl. chemicals)

• *Polymers, fine & specialty chemicals, commodity chemicals, fuel cells*

• *Cycle time to new products, lower cost/higher performance*

? *Scalability, reproducibility, high temp/pressure, kinetics*

An Example: Polyolefin Catalysts



Staff estimates, The Catalyst Group

Catalyst Discovery/Process Issues

Discovery

- *Deposition, Surfaces and Substrates, Temp/Pressure*

Preparation

- *Precipitation, Oxidation, Reduction, Calcination*

Product and Process Development

- *Characterization, Robustness, Lifetime/Regeneration, Scalability*

Analytical Processes: Performance Based

- *Selectivity and yield: new (chip-level?) sensors are needed*
- *"Optical": IR/Raman, UV, photoluminescence, XRD, XAS*
- *"Magnetic": NMR, EPR, mass spectrometry*
- *"Microprobe": AFM, ATM*

Technology Needs: Catalysis Discovery

<u>Design of the Library</u>
- *What makes a catalyst ?*
- *Computational/Modeling*
  - *Structure-Property*
- *Statistics/expert systems*

<u>Synthesis and Processing</u>
- *Automation: 10^3 -10^4 samples*
- *Reproducible results*
- *Order chaos (fewer unknowns)*

<u>Screening</u> (HTS)
- *MEMS Sensors*
- *Process control*
  - *Temperature/pressure*
- *Scalability Predictions*
  - *Interfacial vs. bulk properties*

<u>Cheminformatics</u>
- *Information/Bandwidth*
- *Data integration/analysis*
- *Hardware control*

Discontinuous Innovation & Systems Integration

Hardware Issues: Catalysis Discovery

***SENSORS* (Miniaturization and Mechanical-electrical)**

- Catalyst Selectivity
- Catalytic Turn-over
- Degradation
- Polymer architecture/morphology
- Mechanical Properties

***LIBRARY PROCESSING* (Reproducibility)**

- Control of substrate/sample interfacial properties, diffusion, mass transport
- Control of physical properties (e.g., temperature, time, stress, defects)

***DEPOSITION EQUIPMENT* (Reproducibility)**

- Chemical Vapor Deposition, Plasma Vapor Deposition
- Laser ablation
- Ink jet
- Thermally-driven transport (e-beam, laser, etc.)

Software Issues

Computational

- *Diversity analysis/clustering/analysis*
- *Molecular Modeling--QSAR, QSPR*
- *Reagent Building Block Analysis*
- *Statistics, Design of Experiments*
- *Prediction of Physical Defects, Scalability*

Informatics

- *Indexing*
- *Entity Inventory*
- *Electronic Laboratory Notebook*
- *Search engines/Inferential Engines*
- *Patent and prior art reviews*
- *Literature/Patent Databases*

Decision/Analysis

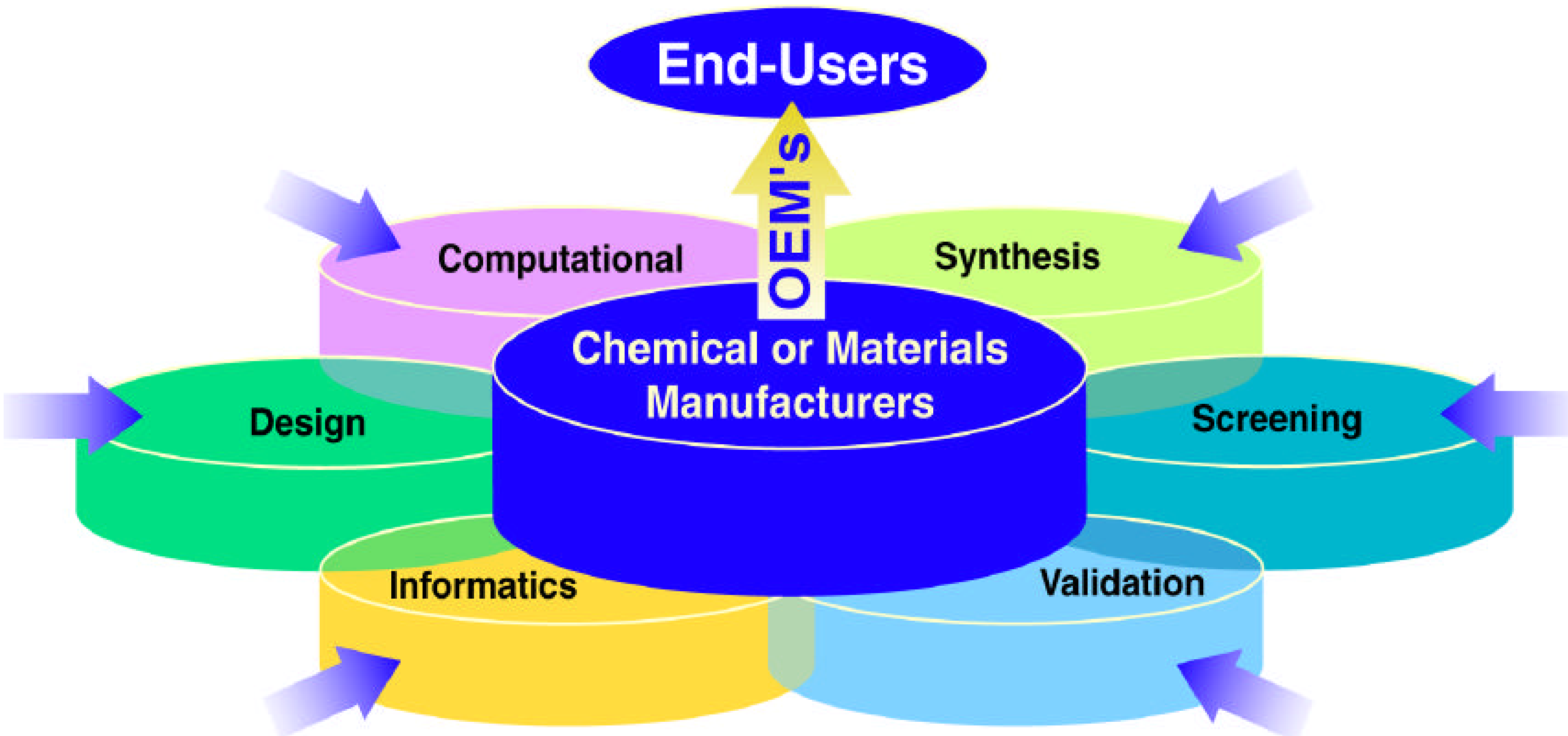
- *Neural Net*
- *Fuzzy Logic*
- *Prediction Tools*

ATP Focused Program Mission

Facilitate the implementation of new research methodologies, within the chemical and advanced materials industries, that will significantly and broadly benefit US society.

Combinatorial Chemistry

ATP Portfolio Strategy



Focused infrastructure on specific applications

Benefits to U.S. Industry

- **Reduced innovation cycle times <u>across organization</u>**
  - *Discovery*
  - *Process development*
  - *Customer service and flexible manufacturing*

- **More efficient use of capital for R&D and manufacturing**
  - *Time-to-market and ROI of R&D $'s*

- **New products/new technologies = new markets**

- **Allows for "out-of-box" experimentation**
  - *Broadens spectrum of materials in development*

The ATP Opportunity

- **Focus base technology innovation toward applications**
- **Bring leading-edge, generic technologies to more industries**
  - *Spur discontinuous innovation in industrial R&D*
  - *Help develop lower-cost hardware and software tools*
  - *Facilitate systems integration: Hardware and software*
- **Improve competitive stance in portfolio industries**
  - *Challenge threats to intellectual property*
  - *Reduced commercialization cycle times*
  - *Permit discovery with "out-of-box" ingredients*